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2-[4-(Trifluoromethyl)phenylsulfanyl]-benzoic acid

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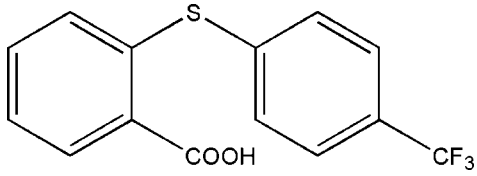
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.054; wR factor = 0.155; data-to-parameter ratio = 12.5.

In the title compound, $C_{14}H_9F_3O_2S$, the dihedral angle between the mean planes of the benzene rings is 88.7 (2)°. The carboxylic acid group is twisted by 13.6 (7)° from the mean plane of its attached aromatic ring. One of the F atoms of the trifluoromethyl group is disordered over two sites in a 0.61 (7):0.39 (7) ratio. In the crystal, inversion dimers linked by pairs of O—H···O hydrogen bonds generate $R_2^2(8)$ loops. Weak C—H···F interactions are also observed.

Related literature

For background to the neuroleptic agent flupentixol (systematic name: (*EZ*)-2-[4-[3-[2-(trifluoromethyl)thioxanthen-9-ylidene]propyl]piperazin-1-yl]ethanol), see: Young *et al.* (1976). For related structures, see: Post *et al.* (1975*a*,*b*); Siddegowda *et al.* (2011*a*,*b*).



Experimental

Crystal data

$C_{14}H_9F_3O_2S$
M_r = 298.28
Triclinic, $P\overline{1}$
a = 7.3071 (5) Å
b = 8.0790 (7) Å
c = 11.3878 (11) Å
α = 82.678 (8)°
β = 83.642 (7)°
γ = 72.309 (7)°
V = 633.41 (10) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 2.63 mm^{-1}
T = 173 K
0.24 × 0.22 × 0.12 mm

Data collection

Agilent Gemini EOS diffractometer
Absorption correction: multi-scan (*CrysAlis PRO* and *CrysAlis RED*; Agilent, 2012)
T_{min} = 0.848, T_{max} = 1.000
3701 measured reflections
2419 independent reflections
2049 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.155
S = 1.04
2419 reflections
193 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.71 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1^{i}	0.82	1.86	2.677 (3)	175
C6—H6···F3^{ii}	0.93	2.59	3.319 (10)	136
C6—H6···F3A^{ii}	0.93	2.50	3.294 (16)	144

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $-x+2, -y+1, -z+2$.

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO* (Agilent, 2012); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SUPERFLIP* (Palatinus & Chapuis, 2007); program(s) used to refine structure: *SHELXL2012* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB7150).

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supplementary materials

Acta Cryst. (2013). E**69**, o1704 [doi:10.1107/S1600536813028778]

2-[4-(Trifluoromethyl)phenylsulfanyl]benzoic acid

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1. Comment

The title compound, (I), is a starting material for the synthesis of flupentixol, a well-documented neuroleptic (Young *et al.*, 1976). The crystal structures of *α*-flupentixol (Post *et al.*, 1975*a*) and *β*-flupentixol (Post *et al.*, 1975*b*) have been reported. As part of our onging studies in this area (Siddegowda *et al.*, 2011*a*,*b*), we now describe the crystal structure of (I).

The dihedral angle between the mean planes of the phenyl rings is 88.7 (2)°. The carboxylic acid group (C2/C1/O2/O1) is twisted by 13.6 (7)° from the mean plane of the adjacent benzene ring (C2–C7). Disorder was modeled over two sets of sites for one fluorine atom (F3), of the trifluoromethyl group with an occupancy ratio of 0.61 (7) : 0.39 (7). In the crystal, O—H···O hydrogen bonds (Table 1) link the molecules into dimers with $R_2^2[8]$ graph-set motifs (Fig. 2). Weak C—H···F interactions are also observed.

2. Experimental

The title compound was obtained as a gift sample from R. L. Fine chemicals, Bengaluru. It was dissolved in 15 ml of mixture of acetonitrile and dimethyl sulphoxide (1:2), stirred for 10 minutes at room temperature. After few days, irregular colourless crystals were formed by slow evaporation of the solvent mixture (m.p: 413-418 K).

3. Refinement

All of the H atoms were placed in their calculated positions and then refined using the riding model with Atom—H lengths of 0.93Å (CH) or 0.82Å (OH). Isotropic displacement parameters for these atoms were set to 1.2 (CH) or 1.5 (OH) times U_{eq} of the parent atom. Disorder was modeled over two sets of sites for one fluorine atom (F3) in the trifluoromethyl group with an occupancy ratio of 0.61 (7) : 0.39 (7). Idealised tetrahderal OH refined as rotating group.

Computing details

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO* (Agilent, 2012); data reduction: *CrysAlis RED* (Agilent, 2012); program(s) used to solve structure: SUPERFLIP (Palatinus & Chapuis, 2007); program(s) used to refine structure: *SHELXL2012* (Sheldrick, 2008); molecular graphics: OLEX2 (Dolomanov *et al.*, 2009); software used to prepare material for publication: OLEX2 (Dolomanov *et al.*, 2009).

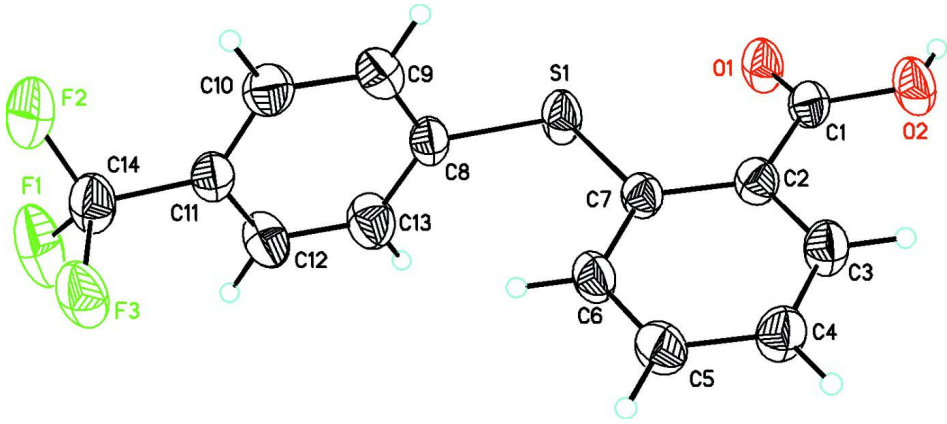

Figure 1

ORTEP drawing of (I) showing 50% probability displacement ellipsoids. Disordered atom, F3A (0.39 (7) occupancy) has been removed for clarity.

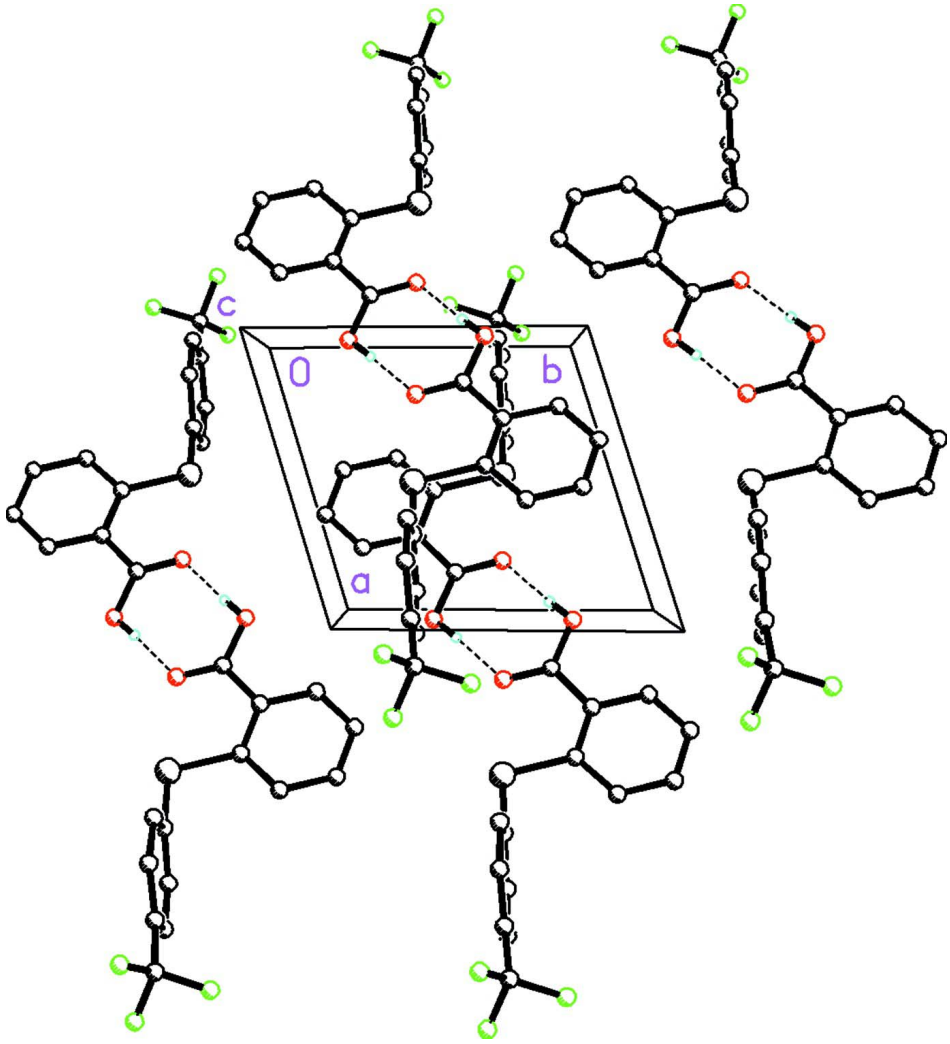

Figure 2

Molecular packing for (I) viewed along the *c* axis. Dashed lines indicate O—H···O intermolecular hydrogen bonds which link the molecules into dimers with $R_2^2[8]$ graph-set motifs and influence the crystal packing. Disordered atom, F3A (0.39 (7) occupancy) and H atoms not involved in hydrogen bonding have been removed for clarity.

2-[4-(Trifluoromethyl)phenylsulfanyl]benzoic acid

Crystal data

$C_{14}H_9F_3O_2S$
$M_r = 298.28$
Triclinic, $P\overline{1}$
$a = 7.3071$ (5) Å
$b = 8.0790$ (7) Å
$c = 11.3878$ (11) Å
$\alpha = 82.678$ (8)°
$\beta = 83.642$ (7)°
$\gamma = 72.309$ (7)°
$V = 633.41$ (10) Å^3
$Z = 2$
$F(000) = 304$
$D_x = 1.564$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 1645 reflections
$\theta = 5.8$–$72.1°$
$\mu = 2.63$ mm^{-1}
$T = 173$ K
Irregular, colourless
0.24 × 0.22 × 0.12 mm

Data collection

Agilent Gemini EOS diffractometer
Radiation source: Enhance (Cu) X-ray Source
Detector resolution: 16.0416 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO* and *CrysAlis RED*; Agilent, 2012)
T_{min} = 0.848, T_{max} = 1.000

3701 measured reflections
2419 independent reflections
2049 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 72.2°, θ_{min} = 5.8°
h = −8→6
k = −9→6
l = −13→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.155
S = 1.04
2419 reflections
193 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0889P)^2 + 0.2312P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.71 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}
Extinction correction: *SHELXL2012* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0044 (14)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	0.51402 (10)	0.35821 (8)	0.70404 (6)	0.0398 (3)	
F1	1.2832 (3)	0.1041 (3)	1.0280 (2)	0.0764 (7)	
F2	1.0648 (3)	0.1392 (4)	1.16595 (19)	0.0849 (8)	
F3	1.1664 (14)	0.3549 (10)	1.0613 (12)	0.054 (2)	0.61 (7)
F3A	1.094 (10)	0.3613 (16)	1.106 (6)	0.100 (14)	0.39 (7)
O1	0.2047 (3)	0.4458 (2)	0.56512 (17)	0.0405 (5)	
O2	−0.0035 (3)	0.7122 (2)	0.54064 (19)	0.0427 (5)	
H2	−0.0646	0.6592	0.5121	0.064*	
C1	0.1620 (4)	0.6021 (3)	0.5733 (2)	0.0332 (5)	
C2	0.2907 (4)	0.6861 (3)	0.6177 (2)	0.0316 (5)	
C3	0.2487 (4)	0.8678 (3)	0.5973 (2)	0.0376 (6)	
H3	0.1387	0.9315	0.5595	0.045*	
C4	0.3668 (4)	0.9550 (3)	0.6319 (2)	0.0396 (6)	
H4	0.3375	1.0757	0.6172	0.048*	
C5	0.5291 (4)	0.8595 (4)	0.6888 (2)	0.0400 (6)	
H5	0.6098	0.9166	0.7125	0.048*	
C6	0.5730 (4)	0.6794 (3)	0.7109 (2)	0.0362 (6)	
H6	0.6825	0.6174	0.7497	0.043*	
C7	0.4555 (3)	0.5897 (3)	0.6759 (2)	0.0303 (5)	

C8	0.6908 (4)	0.3131 (3)	0.8091 (2)	0.0328 (5)
C9	0.6355 (4)	0.3133 (3)	0.9291 (2)	0.0378 (6)
H9	0.5055	0.3396	0.9548	0.045*
C10	0.7722 (4)	0.2748 (4)	1.0114 (2)	0.0405 (6)
H10	0.7343	0.2740	1.0921	0.049*
C11	0.9646 (4)	0.2375 (3)	0.9731 (2)	0.0335 (6)
C12	1.0216 (4)	0.2340 (4)	0.8540 (3)	0.0447 (7)
H12	1.1518	0.2070	0.8288	0.054*
C13	0.8857 (4)	0.2704 (4)	0.7719 (3)	0.0461 (7)
H13	0.9246	0.2663	0.6915	0.055*
C14	1.1122 (4)	0.2104 (4)	1.0605 (3)	0.0450 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0441 (4)	0.0305 (4)	0.0495 (4)	−0.0120 (3)	−0.0242 (3)	−0.0013 (3)
F1	0.0508 (12)	0.0796 (15)	0.0942 (17)	0.0002 (10)	−0.0385 (11)	−0.0105 (12)
F2	0.0770 (15)	0.134 (2)	0.0508 (12)	−0.0459 (15)	−0.0335 (10)	0.0265 (12)
F3	0.057 (5)	0.0356 (19)	0.078 (4)	−0.0181 (19)	−0.034 (4)	−0.002 (2)
F3A	0.15 (3)	0.034 (3)	0.14 (2)	−0.024 (7)	−0.11 (2)	−0.002 (6)
O1	0.0417 (10)	0.0349 (10)	0.0504 (11)	−0.0126 (8)	−0.0228 (8)	−0.0039 (8)
O2	0.0356 (10)	0.0404 (10)	0.0559 (12)	−0.0100 (8)	−0.0219 (8)	−0.0055 (9)
C1	0.0336 (13)	0.0385 (14)	0.0295 (12)	−0.0123 (10)	−0.0104 (10)	0.0000 (10)
C2	0.0343 (13)	0.0335 (12)	0.0293 (12)	−0.0112 (10)	−0.0075 (9)	−0.0039 (9)
C3	0.0381 (13)	0.0339 (13)	0.0410 (14)	−0.0075 (11)	−0.0138 (11)	−0.0026 (10)
C4	0.0456 (15)	0.0300 (13)	0.0460 (15)	−0.0124 (11)	−0.0143 (12)	−0.0016 (11)
C5	0.0415 (15)	0.0410 (15)	0.0452 (15)	−0.0190 (12)	−0.0141 (12)	−0.0055 (11)
C6	0.0331 (13)	0.0373 (14)	0.0412 (14)	−0.0117 (11)	−0.0143 (11)	−0.0019 (11)
C7	0.0308 (12)	0.0316 (12)	0.0302 (12)	−0.0101 (10)	−0.0078 (9)	−0.0023 (9)
C8	0.0339 (12)	0.0267 (12)	0.0393 (13)	−0.0082 (9)	−0.0143 (10)	−0.0009 (10)
C9	0.0317 (13)	0.0391 (14)	0.0441 (15)	−0.0103 (11)	−0.0066 (11)	−0.0067 (11)
C10	0.0466 (15)	0.0464 (16)	0.0333 (13)	−0.0192 (12)	−0.0066 (11)	−0.0041 (11)
C11	0.0387 (13)	0.0219 (11)	0.0424 (14)	−0.0100 (9)	−0.0145 (11)	−0.0005 (9)
C12	0.0320 (13)	0.0542 (17)	0.0466 (16)	−0.0077 (12)	−0.0078 (11)	−0.0086 (13)
C13	0.0395 (15)	0.0595 (18)	0.0365 (14)	−0.0091 (13)	−0.0037 (11)	−0.0071 (13)
C14	0.0550 (18)	0.0317 (13)	0.0538 (17)	−0.0154 (12)	−0.0258 (14)	0.0006 (12)

Geometric parameters (Å, º)

S1—C7	1.782 (2)	C5—H5	0.9300
S1—C8	1.783 (2)	C5—C6	1.387 (4)
F1—C14	1.328 (4)	C6—H6	0.9300
F2—C14	1.322 (4)	C6—C7	1.396 (3)
F3—C14	1.343 (8)	C8—C9	1.381 (4)
F3A—C14	1.35 (2)	C8—C13	1.390 (4)
O1—C1	1.218 (3)	C9—H9	0.9300
O2—H2	0.8200	C9—C10	1.384 (4)
O2—C1	1.324 (3)	C10—H10	0.9300
C1—C2	1.477 (3)	C10—C11	1.378 (4)
C2—C3	1.400 (4)	C11—C12	1.375 (4)

C2—C7	1.404 (3)	C11—C14	1.496 (4)
C3—H3	0.9300	C12—H12	0.9300
C3—C4	1.383 (4)	C12—C13	1.380 (4)
C4—H4	0.9300	C13—H13	0.9300
C4—C5	1.381 (4)		

C7—S1—C8	101.59 (11)	C13—C8—S1	120.6 (2)
C1—O2—H2	109.5	C8—C9—H9	119.7
O1—C1—O2	122.6 (2)	C8—C9—C10	120.5 (2)
O1—C1—C2	123.3 (2)	C10—C9—H9	119.7
O2—C1—C2	114.1 (2)	C9—C10—H10	120.2
C3—C2—C1	118.3 (2)	C11—C10—C9	119.7 (2)
C3—C2—C7	119.4 (2)	C11—C10—H10	120.2
C7—C2—C1	122.3 (2)	C10—C11—C14	120.1 (2)
C2—C3—H3	119.2	C12—C11—C10	120.3 (2)
C4—C3—C2	121.6 (2)	C12—C11—C14	119.5 (3)
C4—C3—H3	119.2	C11—C12—H12	120.0
C3—C4—H4	120.6	C11—C12—C13	120.0 (3)
C5—C4—C3	118.8 (2)	C13—C12—H12	120.0
C5—C4—H4	120.6	C8—C13—H13	119.9
C4—C5—H5	119.7	C12—C13—C8	120.2 (3)
C4—C5—C6	120.7 (2)	C12—C13—H13	119.9
C6—C5—H5	119.7	F1—C14—F3	97.8 (5)
C5—C6—H6	119.5	F1—C14—F3A	122 (3)
C5—C6—C7	121.1 (2)	F1—C14—C11	113.7 (2)
C7—C6—H6	119.5	F2—C14—F1	104.4 (2)
C2—C7—S1	120.83 (18)	F2—C14—F3	115.3 (6)
C6—C7—S1	120.71 (19)	F2—C14—F3A	91 (3)
C6—C7—C2	118.5 (2)	F2—C14—C11	113.2 (2)
C9—C8—S1	120.1 (2)	F3—C14—C11	111.3 (4)
C9—C8—C13	119.2 (2)	F3A—C14—C11	110.3 (8)

S1—C8—C9—C10	178.6 (2)	C8—S1—C7—C2	−165.8 (2)
S1—C8—C13—C12	−179.4 (2)	C8—S1—C7—C6	14.5 (2)
O1—C1—C2—C3	165.0 (3)	C8—C9—C10—C11	0.6 (4)
O1—C1—C2—C7	−13.0 (4)	C9—C8—C13—C12	−2.0 (4)
O2—C1—C2—C3	−13.7 (3)	C9—C10—C11—C12	−1.7 (4)
O2—C1—C2—C7	168.3 (2)	C9—C10—C11—C14	174.9 (2)
C1—C2—C3—C4	−177.4 (2)	C10—C11—C12—C13	1.0 (4)
C1—C2—C7—S1	−2.1 (3)	C10—C11—C14—F1	151.3 (3)
C1—C2—C7—C6	177.6 (2)	C10—C11—C14—F2	32.4 (4)
C2—C3—C4—C5	−0.5 (4)	C10—C11—C14—F3	−99.4 (7)
C3—C2—C7—S1	179.85 (19)	C10—C11—C14—F3A	−68 (4)
C3—C2—C7—C6	−0.4 (4)	C11—C12—C13—C8	0.9 (5)
C3—C4—C5—C6	0.0 (4)	C12—C11—C14—F1	−32.1 (4)
C4—C5—C6—C7	0.3 (4)	C12—C11—C14—F2	−151.0 (3)
C5—C6—C7—S1	179.6 (2)	C12—C11—C14—F3	77.2 (7)
C5—C6—C7—C2	−0.1 (4)	C12—C11—C14—F3A	109 (4)
C7—S1—C8—C9	89.1 (2)	C13—C8—C9—C10	1.2 (4)

C7—S1—C8—C13	−93.5 (2)	C14—C11—C12—C13	−175.6 (3)
C7—C2—C3—C4	0.7 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1^{i}	0.82	1.86	2.677 (3)	175
C6—H6···F3^{ii}	0.93	2.59	3.319 (10)	136
C6—H6···F3*A*^{ii}	0.93	2.50	3.294 (16)	144

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (ii) −*x*+2, −*y*+1, −*z*+2.